Propanamide, 3-phenyl-N-ethyl-N-hept-2-yl-

Inchi: InChI=1S/C18H29NO/c1-4-6-8-11-16(3)19(5-2)18(20)15-14-17-12-9-7-10-13-17/h7,9-10,
InchiKey: SNUPGCCRORSLOI-UHFFFAOYSA-N
Formula: C18H29NO
SMILES: CCCCCC(C)N(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 275.43

Physical Properties

Property code	Value	Unit	Source
gf	192.51	kJ/mol	Joback Method
hf	-228.65	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.437		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	703.79	K	Joback Method
tc	897.76	K	Joback Method
tf	386.44	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.51	J/mol×K	703.79	Joback Method
cpg	741.10	J/mol×K	736.12	Joback Method
cpg	758.61	J/mol×K	768.45	Joback Method
cpg	775.09	J/mol×K	800.78	Joback Method
cpg	790.59	J/mol×K	833.11	Joback Method
cpg	805.16	J/mol×K	865.43	Joback Method
cpg	818.86	J/mol×K	897.76	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume